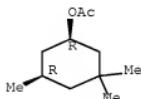


=> d ibib abs hitstr hitind 13 1-3

L3 ANSWER 1 OF 3 HCAPLUS COPYRIGHT 2010 ACS on STN
 ACCESSION NUMBER: 2009:1476435 HCAPLUS Full-text
 TITLE: Essential oil constituents of the rhizomes of
 two types of Curcuma longa of Bangladesh
 AUTHOR(S): Chowdhury, Jasim Uddin; Nandi, Nemai Chandra;
 Bhuiyan, M. Nazrul Islam; Mobarok, M. Hosnay
 CORPORATE SOURCE: BCSIR Laboratories, Chittagong, 4220, Bangladesh
 SOURCE: Bangladesh Journal of Scientific and Industrial
 Research (2008), 43(2), 259-266
 PUBLISHER: Bangladesh Council of Scientific and Industrial
 Research
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Essential oil from the rhizomes of two types of Curcuma longa, yellow and red
 originated in Bangladesh was analyzed by GC-MS. 54 compds. have been
 identified from the yellow type of which the major compds. are ar-tumerone
 (27.78%), tumerone (17.16%), culone (13.82%), 2-carene (4.78%), zingiberene
 (4.37%) and β -sesquiphellandrene (5.57%). The red type contained 39 compds.
 with carvacrol (21.14%), citral (13.91%), methyleugenol (7.31%), geraniol
 (6.99%), menthol (5.11%) and caryophyllene oxide (4.14%) as major
 constituents.
 IT INDEXING IN PROGRESS
 IT 24691-16-5
 RL: BSU (Biological study, unclassified); BIOL (Biological study)
 (cyclohexanol, 3,3,5-trimethyl-, acetate, cis- was present in
 essential oil of rhizome of red but not yellow type Curcuma longa
 of Bangladesh)
 RN 24691-16-5 HCAPLUS
 CN Cyclohexanol, 3,3,5-trimethyl-, 1-acetate, (1R,5R)-rel- (CA INDEX
 NAME)

Relative stereochemistry.



CC 62-2 (Essential Oils and Cosmetics)
 IT 24691-16-5
 RL: BSU (Biological study, unclassified); BIOL (Biological study)
 (cyclohexanol, 3,3,5-trimethyl-, acetate, cis- was present in
 essential oil of rhizome of red but not yellow type Curcuma longa
 of Bangladesh)
 OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS
 RECORD (1 CITINGS)
 REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE
 FOR THIS RECORD. ALL CITATIONS AVAILABLE
 IN THE RE FORMAT

L3 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2010 ACS on STN
 ACCESSION NUMBER: 2005:96462 HCAPLUS Full-text
 DOCUMENT NUMBER: 142:161998
 TITLE: Cis-3,3,5-trimethylcyclohexyl esters for use as
 fragrances
 INVENTOR(S): Kuhn, Walter; Surburg, Horst
 PATENT ASSIGNEE(S): Symrise GmbH & Co. Kg, Germany
 SOURCE: PCT Int. Appl., 33 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
-----	----	-----	-----	-----
WO 2005009492	A1	20050203	WO 2004-EP51292	200406 30
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW	RN: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG	DE 10332908	A1 20050210	DE 2003-10332908 200307 19
DE 10332908	A1	20050210	DE 2003-10332908	200307 19
EP 1648526	A1	20060426	EP 2004-741922	200406 30
EP 1648526	B1	20090909		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK	AT 442166	T 20090915	AT 2004-741922	200406 30
US 20060211597	A1	20060921	US 2006-565241	200601 19
PRIORITY APPLN. INFO.:			DE 2003-10332908	A 200307 19
			WO 2004-EP51292	W 200406 30

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

OTHER SOURCE(S): MARPAT 142:161998

AB The invention relates to mixts. of cis-3,3,5-trimethylcyclohexyl esters with trans-3,3,5-trimethylcyclohexyl esters, the use of cis-3,3,5-trimethylcyclohexyl esters as fragrances and individual cis-3,3,5-

trimethylcyclohexyl esters and their use as fragrances. Thus 3,3,5-trimethylcyclohexyl acetate was synthesized from 3,3,5-trimethylcyclohexanol and acetic acid anhydride; the product contained 90% cis-3,3,5-trimethylcyclohexyl acetate. It was used in a fragrance composition as 65 weight part ingredient; other components were (weight parts): benzyl acetate 30; Ozonil (2-Tridecenitrile) 10% in diethylphthalate 5; dihydromyrcenol 150; decanal 1; 2-phenoxyethylisobutyrate 100; methylcedrylketone 35; hexyl cinnamic aldehyde 50; Lilial 30; linalyl acetate 100; Galaxolide 50% in diethylphthalate 10; cedryl acetate 30; Zibeth absolute synth. 1; lemon terpene 70; ethylvanillin 3; γ -undecalactone 1; citronitrile 10; Projasmon P (2-heptylcycloheptanon) 1; Agrumex HC (2-*tert*-butylcyclohexyl acetate) 30; hexenyl isobutyrate, cis/trans- 1; hexenylacetate cis/trans- 1; Limette oil, synth. 10; diethylphthalate 2.66.

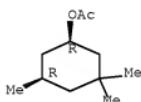
IT 24691-16-5P

RL: COS (Cosmetic use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(cis-3,3,5-trimethylcyclohexyl esters for use as fragrances)

RN 24691-16-5 HCAPLUS

CN Cyclohexanol, 3,3,5-trimethyl-, 1-acetate, (1R,5R)-rel- (CA INDEX NAME)

Relative stereochemistry.



IPCI A61L0009-01 [ICM,7]; C07C0069-06 [ICS,7]; C07C0069-00 [ICS,7,C*]

IPCR C07C0069-00 [I,C*]; C07C0069-013 [I,A]

CC 62-2 (Essential Oils and Cosmetics)

IT 24691-16-5P 24691-18-7P 60234-70-0P 60234-71-1P

828912-37-4P 828912-38-5P 828912-39-6P 828912-40-9P

828912-41-0P 828912-42-1P 828912-44-3P 828912-46-5P

828912-48-7P

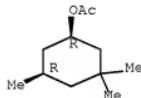
RL: COS (Cosmetic use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(cis-3,3,5-trimethylcyclohexyl esters for use as fragrances)

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1970:465956 HCAPLUS [Full-text](#)
DOCUMENT NUMBER: 73:65956
ORIGINAL REFERENCE NO.: 73:10799a,10802a
TITLE: Reductions with metal-ammonia combinations. II.
Monothioacetals and monothioketals. Synthesis
of alkoxymercaptans
AUTHOR(S): Eliel, Ernest L.; Doyle, Terrence W.
CORPORATE SOURCE: Dep. of Chem., Univ. of Notre Dame, Notre Dame,
IN, USA
SOURCE: Journal of Organic Chemistry (1970), 35(8),
2716-22
CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 73:65956
 AB The reduction of oxathiolanes and oxathianes with metal-liquid NH₃ combinations gives rise to β - and γ -alkoxymercaptans. Twenty-six cases were studied; yields are good for all oxathianes and most oxathiolanes (except those with very simple 2-alkyl groups) when the metal is Ca.
 IT 24691-16-5P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 24691-16-5 HCPLUS
 CN Cyclohexanol, 3,3,5-trimethyl-, 1-acetate, (1R,5R)-rel- (CA INDEX NAME)

Relative stereochemistry.



CC 23 (Aliphatic Compounds)
 IT 176-38-5P 4332-51-8P 5721-87-9P 10160-69-7P 10160-71-1P
 10160-72-2P 10160-73-3P 10160-74-4P 10160-75-5P 10160-76-6P
 10160-77-7P 10160-78-8P 16047-98-6P 16047-99-7P 17642-75-0P
 17642-77-2P 17642-78-3P 17643-69-5P 17643-70-8P 24691-15-4P
 24691-16-5P 24691-17-6P 24691-18-7P 24691-19-8P
 24691-20-1P 24691-50-7P 24691-51-8P 24699-49-8P 24699-55-6P
 24699-57-8P 24699-59-0P 24699-60-3P 24699-61-4P 24699-65-8P
 24699-66-9P 24699-76-1P 24699-77-2P 24699-78-3P 24699-79-4P
 24699-80-7P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 OS.CITING REF COUNT: 9 THERE ARE 9 CAPLUS RECORDS THAT CITE THIS RECORD (9 CITINGS)

=> d ibib abs hitstr hitind 14 1-8

L4 ANSWER 1 OF 8 HCPLUS COPYRIGHT 2010 ACS on STN
 ACCESSION NUMBER: 2009:756097 HCPLUS Full-text
 DOCUMENT NUMBER: 151:85996
 TITLE: Use of 2,4'-dimethyl-propiophenone as a fragrance substance
 INVENTOR(S): Kuhn, Walter; Lambrecht, Stefan; Panten, Johannes; Wiedmann, Willi
 PATENT ASSIGNEE(S): Symrise G.m.b.H. & Co. K.-G., Germany
 SOURCE: Eur. Pat. Appl., 22pp.
 CODEN: EPXWDW
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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 EP 2072083 A1 20090624 EP 2007-123731
 200712
 19
 R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU,
 IE, IS, IT, LI, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI,
 SK, TR, AL, BA, HR, MK, RS
 US 20090162308 A1 20090625 US 2008-337751
 200812
 18
 PRIORITY APPLN. INFO.: EP 2007-123731 A
 200712
 19

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

OTHER SOURCE(S): CASREACT 151:85996

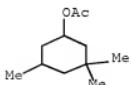
AB The invention concerns the use of 2,4'-dimethylpropiophenone as a fragrance substance, preferably as a fragrance substance for imparting, modifying and/or reinforcing one, two, three or all the odor notes floral, rosy, rose oxide-like and herbal-like, preferably both of the odor notes rose oxide-like and herbal-like. Perfume, shampoo, antiperspirant, hair cosmetic and detergent compns. are exemplified that contain 2,4'-dimethyl-propiophenone as fragrance. Thus toluene and isobutyric acid chloride were reacted in the presence of aluminum chloride to obtain 2,4'-dimethyl-propiophenone with an isomer distribution of 94.4% para, 1.7 meta and 3.8 ortho isomer. A perfume composition contained (g): n-dodecanal 3; 2-methylundecanal 7; vertocitral 10; galbanum resin 3; styrolyl acetate 7; terpinylacetate 30; citral 10; Italian orange oil 20; Claritone 10; petit grain oil 20; lavandin oil 100; spikenard oil 100; rosemary oil 60; Spanish sage oil 30; dill oil 10; mugwort oil 10; Lyral 50; Hedione 50; methyloctane carbonate 1; Herbaflorate 25; herbylpropionate 20; Iso E Super 70; vetiver oil 10; veticol acetate 5; patchouly oil 30; Evernyl 5; Ambroxid crystalline 4; 2,4'-di-Me-propiophenone 70; dipropylene glycol 230.

IT 67859-96-5

RL: COS (Cosmetic use); BIOL (Biological study); USES (Uses)
 (in combination with; use of 2,4'-di-Me-propiophenone as a
 fragrance substance)

RN 67859-96-5 HCPLUS

CN Cyclohexanol, 3,3,5-trimethyl-, 1-acetate (CA INDEX NAME)



IPCI A61Q0005-00 [I,A]; C11B0009-00 [I,A]; C07C0049-76 [I,A]; C07C0049-00 [I,C*]

IPCR A61Q0005-00 [I,C]; A61Q0005-00 [I,A]; C07C0049-00 [I,C]; C07C0049-76 [I,A]; C11B0009-00 [I,C]; C11B0009-00 [I,A]

CC 62-5 (Essential Oils and Cosmetics)

Section cross-reference(s): 5, 66

IT 60-12-8, 2-Phenylethyl alcohol 76-22-2, Camphor 78-69-3,
 Tetrahydrolinalool 78-70-6, Linalool 80-54-6,
 2-Methyl-3-(4-tert-butylphenyl)propanal 87-44-5, Caryophyllene
 88-41-5, 2-tert-Butylcyclohexyl acetate 90-17-5,

α -Trichloromethylbenzyl acetate 91-64-5, Coumarin 94-47-3,
 Phenylethylbenzoate 94-48-4, Geranylbenzoate 97-89-2,
 Citronellylisobutyrate 101-48-4, Phenylacetaldehyde dimethyl
 acetal 101-81-5, Diphenylmethane 101-84-8, Diphenyl oxide
 101-86-0, α -Hexylcinnamic aldehyde 102-20-5,
 Phenylethylphenyl acetate 103-45-7 103-48-0 103-52-6
 103-60-6, 2-Phenoxyethylisobutyrate 104-54-1, Cinnamic alcohol
 104-62-1 105-85-1, Citronellyl formate 105-86-2, Geranyl formate
 105-87-3, Geranyl acetate 105-90-8, Geranylpropionate 105-95-3,
 Ethylenebrassylate 106-02-5, Oxacyclohexadecan-2-one 106-21-8
 106-22-9, Citronellol 106-24-1, Geraniol 106-25-2, Nerol
 106-29-6, Geranylbutyrate 106-72-9, 2,6-Dimethyl-5-hepten-1-al
 109-20-6, Geranylisovalerate 112-31-2, Decanal 112-43-6,
 10-Undecenol 112-45-8, 10-Undecenal 115-95-7, Linalyl acetate
 118-58-1, Benzylsalicylate 119-61-9, Benzenophenone, biological
 studies 121-33-5, Vanillin 122-40-7 122-70-3,
 Phenylethylpropionate 122-78-1, Phenylacetaldehyde 127-41-3,
 α -Ionone 127-51-5, α -Isomethylionone 140-26-1,
 Phenylethylisovalerate 141-14-0, Citronellylpropionate 141-16-2,
 Citronellylbutyrate 150-84-5, Citronellyl acetate 470-82-6,
 1,8-Cineole 498-16-8, Lavandulol 502-61-4, Farnesene 507-70-0,
 Borneol 562-74-3, 4-Terpinenol 1205-17-0,
 2-Methyl-3-(4-methylenedioxyphenyl)propanal 1817-90-9
 1860-40-8 2345-26-8, Geranylisobutyrate 2500-83-6 2565-82-4,
 Geranyl methyl ether 2630-39-9, Methyldihydrojasmonate 3391-86-4,
 1-Octen-3-ol 3558-60-9 3681-71-8, cis-3-Hexenyl acetate
 3681-82-1, trans-3-Hexenylacetate 3796-70-1, Geranylacetone
 4602-84-0, Farnesol 4707-47-5 4941-78-0,
 Oxacyclohexadec-13-en-2-one 5413-60-5,
 4,7-Methano-3a,4,5,6,7,7a-hexahydro-6-indenyl acetate 6259-76-3,
 Hexylsalicylate 6315-04-4 7212-44-4, Nerolidol 7492-67-3,
 Citronellyloxyacetalddehyde 7779-30-8 7785-33-3, Geranyl tiglate
 8000-41-7, Terpineol 8007-35-0, Terpinyl acetate 10339-55-6,
 Ethyllinalool 10482-77-6, Citronellylbenzoate 10522-41-5
 13019-22-2, 9-Decenol 16409-43-1, Roseoxide 20777-39-3,
 Lavandulyl acetate 21145-77-7 21944-94-5 23726-91-2,
 β -Damascone 23726-93-4, β -Damascenone 24717-85-9,
 Citronellyl tiglate 25225-10-9 25634-93-9,
 2-Methyl-5-phenylpentanol 28069-72-9, trans-2,cis-6-Nonadienol
 28219-61-6, 2-Ethyl-4-(2,2,3-trimethyl-3-cyclopenten-1-yl)-2-butene-1-
 ol 28940-11-6 31906-04-4,
 4-(4-Hydroxy-4-methylpentyl)-3-cyclohexenecarboxaldehyde
 32210-23-4, 4-tert-Butylcyclohexyl acetate 32539-78-9,
 Oxacyclohexadec-12-en-2-one 33673-71-1 35087-49-1,
 γ -Damascone 36613-11-3 41199-19-3 43052-87-5,
 α -Damascone 50816-18-7, 9-Decenyl acetate 53219-21-9,
 Dihydromyrcenol 54464-57-2 54546-26-8,
 2-Butyl-4,4,6-trimethyl-1,3-dioxane 55066-48-3,
 3-Methyl-5-phenylpentanol 55719-85-2, 2-Phenylethyl tiglate
 56011-02-0, Phenylethylisoamyl ether 57378-68-4, δ -Damascone
 63500-71-0 64988-06-3 67634-15-5,
 3-(4-Ethylphenyl)-2,2-dimethylpropanal 67662-96-8, Phenethyl
 pivalate 67859-96-5 68039-49-6,
 2,4-Dimethyl-3-cyclohexenecarboxaldehyde 68527-77-5 68922-10-1,
 Citronellylisovalerate 70024-54-3 74338-72-0,
 2,4,4,7-Tetramethyloct-6-en-3-one 101151-17-1 125109-85-5,
 3-(3-Isopropylphenyl)butanal 135546-43-9 145206-68-4
 RL: COS (Cosmetic use); BIOL (Biological study); USES (Uses)
 (in combination with; use of 2,4'-di-Me-propiophenone as a

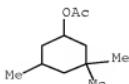
fragrance substance)

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR
THIS RECORD. ALL CITATIONS AVAILABLE IN
THE RE FORMAT

L4 ANSWER 2 OF 8 HCPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2009:46762 HCPLUS Full-text
DOCUMENT NUMBER: 150:128383
TITLE: Use of methyl methyl ether and additional
ethers to provide a feeling of cleanliness and
purity especially with deodorants
INVENTOR(S): Kurzenne, Pierre; Collas, Violaine; Favre-Bulle,
Beatrice; Machinek, Arnold; Surburg, Horst
PATENT ASSIGNEE(S): Symrise G.m.b.H. & Co. K.-G., Germany
SOURCE: Eur. Pat. Appl., 32pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 2014273	A1	20090114	EP 2007-110259	200706 14
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, MK, RS			EP 2007-110259	200706 14
PRIORITY APPLN. INFO.:				

OTHER SOURCE(S): MARPAT 150:128383
 AB The invention concerns the use of a methyl Me ether or a mixture of two or
 more methyl ethers in cosmetic formulations in order to improve the feeling
 of cleanliness and purity. Thus a composition contained (weight parts): L-
 menthylmethyl ether 200; Florazon 10; Frescomenthe 30; peppermint oil 10; L-
 menthol 200; L-carvone 10; Calone 1951 1; Hedione 50; Anethol 5; Iso E Super
 100; Ambrinol S 3; isomethyl acetate 50; dipropylene glycol 330.
 IT 67859-96-5
 RL: COS (Cosmetic use); BIOL (Biological study); USES (Uses)
 (in combination with; use of methyl Me ether and addnl. ethers
 to provide a feeling of cleanliness and purity especially with
 deodorants)
 RN 67859-96-5 HCPLUS
 CN Cyclohexanol, 3,3,5-trimethyl-, 1-acetate (CA INDEX NAME)



IPCI A61K0008-04 [I,A]; A61K0008-33 [I,A]; A61K0008-30 [I,C*];
 A61Q0013-00 [I,A]; A61Q0015-00 [I,A]

CC 62-4 (Essential Oils and Cosmetics)
 IT 78-69-3, Tetrahydrodrolinalool 80-54-6,
 2-Methyl-3-(4-tert-butylphenyl)propanal 88-41-5,
 2-tert-Butylcyclohexyl acetate 91-64-5, Coumarin 101-86-0,
 α -Hexylcinnamic aldehyde 103-60-6, 2-Phenoxyethylisobutyrate
 104-54-1, Cinnamic alcohol 105-95-3, Ethylenebrassyate
 106-02-5, Oxacyclohexadecan-2-one 106-22-9, Citronellol 106-72-9
 115-95-7, Linalyl acetate 118-58-1, Benzylsalicylate 121-33-5,
 Vanillin 122-40-7 127-41-3, α -Ionone 127-51-5,
 α -Isomethylionone 1205-17-0 1222-05-5, Galaxolide
 2500-83-6 2630-39-9, Methyldihydrojasmonate 3681-71-8,
 cis-3-Hexenyl acetate 3681-82-1, trans-3-Hexenyl acetate
 4941-78-0, Oxacyclohexadec-13-en-2-one 5413-60-5, Herbaflorat
 6259-76-3, Hexylsalicylate 7779-30-8 8007-35-0, Terpinyl acetate
 10339-55-6, Ethylalool 10522-41-5 14765-30-1,
 2-sec-Butylcyclohexanone 21145-77-7 21944-94-5 22457-23-4
 28069-72-9, trans-2,cis-6-Nonadienol 28219-61-6,
 2-Ethyl-4-(2,2,3-trimethyl-3-cyclopenten-1-yl)-2-buten-1-ol
 28940-11-6 32210-23-4, 4-tert-Butylcyclohexyl acetate
 32539-78-9, Oxacyclohexadec-12-en-2-one 41199-19-3 53219-21-9,
 Dihydromyrcenol 54464-57-2 54464-57-2, Iso E Super 63500-71-0
 67634-15-5, 3-(4-Ethylphenyl)-2,2-dimethylpropanal 67715-80-4,
 2-Methyl-4-propyl-1,3-oxathiane 67859-96-5 68039-49-6,
 2,4-Dimethyl-3-cyclohexenecarboxaldehyde 74338-72-0 101151-17-1
 125109-85-5 130066-44-3, Lyral
 RL: COS (Cosmetic use); BIOL (Biological study); USES (Uses)
 (in combination with; use of menthyl Me ether and addnl. ethers
 to provide a feeling of cleanliness and purity especially with
 deodorants)

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR
 THIS RECORD. ALL CITATIONS AVAILABLE IN
 THE RE FORMAT

L4 ANSWER 3 OF 8 HCPLUS COPYRIGHT 2010 ACS on STN
 ACCESSION NUMBER: 2008:1243858 HCPLUS Full-text
 DOCUMENT NUMBER: 149:424509
 TITLE: Cooling compositions including menthyl esters
 INVENTOR(S): Kiefer, Jesse; Harvey, Joan E.
 PATENT ASSIGNEE(S): Cadbury Adams USA LLC, USA
 SOURCE: PCT Int. Appl., 53pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

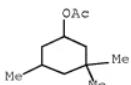
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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-----	A1	20081016	WO 2008-US59530	200804
				07

W: AE, AG, AL, AM, AO, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY,
 BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE,
 EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN,
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 NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK,
 SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC,

VN, ZA, ZM, ZW
 RN: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HR,
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 TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
 US 20070221236 A1 20070927 US 2007-732942 200704
 05
 EP 2129234 A1 20091209 EP 2008-745205 200804
 07
 R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HR,
 HU, IE, IS, IT, LI, LT, LU, LV, MC, MT, NL, NO, PL, PT, RO,
 SE, SI, SK, TR
 PRIORITY APPLN. INFO.: US 2007-732942 A 200704
 05
 US 2005-723698P P 200510
 05
 US 2006-543473 A2 200610
 05
 WO 2008-US59530 W 200804
 07

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

AB Cooling compns. deliver a prolonged physiol. cooling sensation to the skin or a mucous membrane. The cooling compns. may be present alone or in product such as a chewing gum or a confection. In some embodiments, the cooling compns. include menthyl glutarate and at least one addnl. cooling agent, which may be WS-3 or WS-23, and optionally menthol. The cooling compns. may be in a liquid form at room temperature. Thus, a cooling composition includes menthyl glutarate 5-60, WS3 or WS23 5-50, and menthol 15-85 % weight/weight
 IT 67859-96-5
 RL: FFD (Food or feed use); BIOL (Biological study); USES (Uses)
 (cooling compns. including menthyl esters and chewing gums comprising these)
 RN 67859-96-5 HCAPLUS
 CN Cyclohexanol, 3,3,5-trimethyl-, 1-acetate (CA INDEX NAME)



IPC1 A23G0004-00 [I,A]; A23G0004-18 [I,A]; A61K0009-68 [I,A]
 IPCR A23G0004-00 [I,C]; A23G0004-00 [I,A]; A23G0004-18 [I,C]; A23G0004-18
 [I,A]; A61K0009-68 [I,C]; A61K0009-68 [I,A]
 CC 17-6 (Food and Feed Chemistry)
 IT 89-78-1 89-79-2 1490-04-6D, esters 2623-23-6 16409-45-3

17162-29-7 34212-59-4 39711-79-0 42822-86-6 51115-67-4
 67859-96-5 77304-30-4 77341-67-4 185915-25-7
 220621-22-7 930287-43-7

RL: FFD (Food or feed use); BIOL (Biological study); USES (Uses)
 (cooling compns. including menthyl esters and chewing gums
 comprising these)

OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)
 REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 8 HCAPLUS COPYRIGHT 2010 ACS on STN
 ACCESSION NUMBER: 2007:1093006 HCAPLUS [Full-text](#)
 DOCUMENT NUMBER: 147:384825
 TITLE: Cooling compositions including menthyl esters
 INVENTOR(S): Kiefer, Jesse; Harvey, Joan E.
 PATENT ASSIGNEE(S): Cadbury Adams USA LLC., USA
 SOURCE: U.S. Pat. Appl. Publ., 20pp., Cont.-in-part of U.S. Ser. No. 543,473.
 CODEN: USXXCO
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20070221236	A1	20070927	US 2007-732942	20070405
AU 2006302337	A1	20070419	AU 2006-302337	20061005
CA 2623545	A1	20070419	CA 2006-2623545	20061005
WO 2007044526	A2	20070419	WO 2006-US39158	20061005

WO 2007044526 A3 20070628
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 MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG,
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EP 1962779	A2	20080903	EP 2006-825560	20061005
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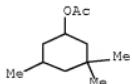
1796

JP 2009519003	T	20090514	JP 2008-534717	
				200610 05
IN 2008KN01197	A	20080905	IN 2008-KN1197	
				200803 24
MX 2008004307	A	20080409	MX 2008-4307	
				200803 31
CN 101282707	A	20081008	CN 2006-80037226	
				200804 07
WO 2008124667	A1	20081016	WO 2008-US59530	
				200804 07
W: AE, AG, AL, AM, AO, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, NO, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GO, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
EP 2129234	A1	20091209	EP 2008-745205	
				200804 07
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PRIORITY APPLN. INFO.:			US 2005-723698P	P
				200510 05
			US 2006-543473	A2
				200610 05
			WO 2006-US39158	W
				200610 05
			US 2007-732942	A
				200704 05
			WO 2008-US59530	W
				200804 07

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

AB Cooling compns. deliver a prolonged physiol. cooling sensation to the skin or a mucous membrane. The cooling compns. may be present alone or in product such as a chewing gum or a confection. In some embodiments, the cooling compns. include methyl glutarate and at least one addnl. cooling agent, which may be WS-3 or WS-23, and optionally menthol. The cooling compns. may be in a

liquid form at room temperature. Thus, a cooling composition includes menthyl glutarate 5-60, WS3 or WS23 5-50, and menthol 15-85 % weight/weight
 IT 67859-96-5, Homomenthyl acetate
 RL: FFD (Food or feed use); BIOL (Biological study); USES (Uses)
 (cooling compns. including menthyl esters and chewing gums comprising these)
 RN 67859-96-5 HCPLUS
 CN Cyclohexanol, 3,3,5-trimethyl-, 1-acetate (CA INDEX NAME)



INCL 131352000
 IPCI A24B0015-00 [I,A]
 IPCR A24B0015-00 [I,C]; A24B0015-00 [I,A]
 NCL 131/352.000
 CC 17-6 (Food and Feed Chemistry)
 IT 89-78-1, Menthol 89-79-2, L-Isopulegol 1490-04-6D, Menthol,
 esters 2623-23-6, L-Menthyl acetate 16409-45-3, Menthyl acetate
 17162-29-7, Menthyl lactate 34212-59-4 39711-79-0, WS-3
 42822-86-6, p-Menthane-3,8-diol 51115-67-4, WS-23
 67859-96-5, Homomenthyl acetate 77304-30-4 77341-67-4
 185915-25-7, L-Menthyl lactate 220621-22-7 930287-43-7
 RL: FFD (Food or feed use); BIOL (Biological study); USES (Uses)
 (cooling compns. including menthyl esters and chewing gums comprising these)

L4 ANSWER 5 OF 8 HCPLUS COPYRIGHT 2010 ACS on STN
 ACCESSION NUMBER: 2001:452890 HCPLUS Full-text
 DOCUMENT NUMBER: 135:66066
 TITLE: Ester odor neutralizers
 INVENTOR(S): Rohde, Ute; Hillers, Stephan; Surburg, Horst;
 Sonnenberg, Steffen; Mcdermott, Keith; Smith,
 Leslie; Sparkuhle, Karl
 PATENT ASSIGNEE(S): Haarmann & Reimer G.m.b.H., Germany; Haarmann
 und Reimer G.m.b.H.
 SOURCE: PCT Int. Appl., 52 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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WO 2001043784	A2	20010621	WO 2000-EP12374	2000012 08
WO 2001043784	A3	20011115		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH,
 CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH,
 GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK,
 LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ,

PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ,
UA, UG, US, UZ, VN, YU, ZA, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH,
CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE,
TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD,
TG

EP 1239890	A2	20020918	EP 2000-991148	
				2000012
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EP 1239890	B1	20041110		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2003516813	T	20030520	JP 2001-544920	
				2000012
				08
AT 281847	T	20041115	AT 2000-991148	
				2000012
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ES 2231305	T3	20050516	ES 2000-991148	
				2000012
US 20030068295	A1	20030410	US 2002-149564	
				200209
				09
US 7157411	B2	20070102		
PRIORITY APPLN. INFO.:			US 1999-170424P	P
				199912
				13
			WO 2000-EP12374	W
				2000012
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ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

OTHER SOURCE(S): MARPAT 135:66066

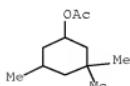
AB This invention relates to odor neutralizers comprising esters such as 2,4-dimethyl-3-pentyl esters of propionic, isobutyric, crotonic, and butyric acids. These esters and a number of other similar esters were prepared and tested for their deodorant properties against sweat, ammonia, tobacco smoke, etc.

IT 67859-96-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BUU (Biological use, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(ester odor neutralizers)

RN 67859-96-5 HCAPLUS

CN Cyclohexanol, 3,3,5-trimethyl-, 1-acetate (CA INDEX NAME)



A61K0008-30 [I,A]; A61K0008-37 [I,A]; A61L0009-01 [I,C*];
 A61L0009-01 [I,A]; A61Q0005-00 [I,C*]; A61Q0005-00 [I,A];
 A61Q0005-10 [I,C*]; A61Q0005-10 [I,A]; A61Q0007-00 [I,C*];
 A61Q0007-00 [I,A]; A61Q0009-04 [I,C*]; A61Q0009-04 [I,A];
 A61Q0015-00 [I,C*]; A61Q0015-00 [I,A]; C02F0001-00 [I,C*];
 C02F0001-00 [I,A]; C11D0003-20 [I,C*]; C11D0003-20 [I,A]

CC 62-5 (Essential Oils and Cosmetics)

Section cross-reference(s): 23

IT 1637-22-5P 1637-24-7P 6070-14-0P 20777-45-1P 32376-43-5P

65466-77-5P 67859-96-5P 87386-67-2P 94021-79-1P

94200-12-1P 97766-62-6P 105937-88-0P 119617-64-0P

123232-56-4P 141553-01-7P 345288-58-6P 345288-59-7P

345288-60-0P 345288-61-1P 345288-62-2P 345288-63-3P

345288-64-4P 345288-65-5P 345288-66-6P 345288-67-7P

345288-68-8P 345288-69-9P 345288-70-2P 345288-71-3P

345288-72-4P 345288-73-5P 345288-74-6P 345288-75-7P

345288-76-8P 345288-77-9P 345288-78-0P 345288-79-1P

345288-80-4P 345288-81-5P 345288-82-6P 345288-83-7P

RL: BAC (Biological activity or effector, except adverse); BSU
 (Biological study, unclassified); BUU (Biological use,
 unclassified); SPN (Synthetic preparation); BIOL (Biological study);
 PREP (Preparation); USES (Uses)
 (ester odor neutralizers)

OS.CITING REF COUNT: 8 THERE ARE 8 CAPLUS RECORDS THAT CITE THIS
 RECORD (8 CITINGS)

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR
 THIS RECORD. ALL CITATIONS AVAILABLE IN
 THE RE FORMAT

L4 ANSWER 6 OF 8 HCPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 1986:33872 HCPLUS Full-text

DOCUMENT NUMBER: 104:33872

ORIGINAL REFERENCE NO.: 104:5553a,5556a

TITLE: Ultraviolet absorbing compounds and compositions
 containing these compounds

INVENTOR(S): Baker, James Albert

PATENT ASSIGNEE(S): Graesser Laboratories Ltd., UK

SOURCE: Eur. Pat. Appl., 25 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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EP 153089	A1	19850828	EP 1985-300800	198502 06
R: AT, BE, CH, DE, FR, IT, LI, LU, NL, SE				
GB 2155467	A	19850925	GB 1985-3039	198502 06
GB 2155467	B	19870325		
US 4592906	A	19860603	US 1985-699955	198502 08
AU 8538675	A	19850822	AU 1985-38675	198502

ZA 8501081	A	19861029	ZA 1985-1081	13
				198502
				13
JP 60231637	A	19851118	JP 1985-27539	198502
				14
PRIORITY APPLN. INFO.:			GB 1984-3836	A
				198402
				14

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT
 OTHER SOURCE(S): MARPAT 104:33872

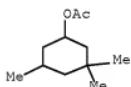
AB 4-Me2NC6H4CH:CHCO2R (I; R = 2-ethylhexyl, 2-octyl) were prepared for use as UV (type A) absorbers in sunscreen compns. Thus, 40 g I (R = Et), 60 mL 2-ethylhexanol, 60 mL PhMe, and 0.1 g Na were stirred at 130° to give, after workup and vacuum distillation, 38 g I (R = 2-ethylhexyl; II). II has a m.p. of -5°, is completely miscible with both mineral oil and MeOH, and has an absorptivity of 101 at λ_{max} = 363 nm. Several sun-block formulations were given.

IT 67859-96-5

RL: RCT (Reactant); RACT (Reactant or reagent)
 (condensation of, with dimethylaminobenzaldehyde)

RN 67859-96-5 HCAPLUS

CN Cyclohexanol, 3,3,5-trimethyl-, 1-acetate (CA INDEX NAME)



IPCI C07C0101-46 [ICM, 4]; A61K0007-42 [ICS, 4]

IPCR C09K0003-00 [I,C*]; C09K0003-00 [I,A]; A61K [I,S]; A61K0008-00 [I,C*]; A61K0008-00 [I,A]; A61K0008-30 [I,C*]; A61K0008-37 [I,A]; A61K0008-41 [I,A]; A61K0008-44 [I,A]; A61K0031-185 [I,C*]; A61K0031-195 [I,A]; A61Q0017-04 [I,C*]; A61Q0017-04 [I,A]; C07C0067-00 [I,C*]; C07C0067-00 [I,A]; C07C0227-00 [I,C*]; C07C0227-00 [I,A]; C07C0229-00 [I,C*]; C07C0229-44 [I,A]

CC 25-18 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
 Section cross-reference(s): 62

IT 112-06-1 112-14-1 112-17-4 123-92-2 2051-50-5 58430-94-7
 67859-96-5

RL: RCT (Reactant); RACT (Reactant or reagent)
 (condensation of, with dimethylaminobenzaldehyde)

OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD (2 CITINGS)

L4 ANSWER 7 OF 8 HCAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 1959:94508 HCAPLUS Full-text

DOCUMENT NUMBER: 53:94508

ORIGINAL REFERENCE NO.: 53:17008i,17009a-d

TITLE: Stereochemistry of the dihydroisophorols

AUTHOR(S): Alkonyi, Istvan

CORPORATE SOURCE: Univ. Leipzig, Germany

SOURCE: Chemische Berichte (1959), 92, 1130-4

CODEN: CHBEAM; ISSN: 0009-2940

DOCUMENT TYPE:

Journal

LANGUAGE:

Unavailable

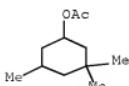
AB The dihydroisophorol (I), m. 34°, and the isomer (II), m. 56°, were identified chemically and spectroscopically as the cis and trans isomers, resp. The compound regarded by Knoevenagel [Ann. 297, 194(1897)] as I was identified as an acetylated product. I (7.6 g.) and 1.23 g. Na in 20 cc. C6H6 refluxed 2 hrs., treated with 7.6 g. phthalic anhydride (III) in 100 cc. C6H6, refluxed 5 hrs., poured into H2O acidified with HCl, and extracted with Et2O, the extract dried and evaporated, and the residue recrystd. from C6H6 and then EtOH gave 2.5 g. I acid phthalate (IV), m. 129°. II (10 g.) and 10 g. III in 30 cc. C6H6 refluxed 6.5 hrs., cooled, filtered from 1.6 g. unchanged III, and evaporated yielded 15.2 g. II acid phthalate (V), m. 120-1° (EtOH). I treated with Ac2O and KOAc gave the acetate (VI), b27 96-7°, n1D 1.4411, d19 0.9197. VI yielded similarly the acetate (VII), b24 98-8.5°, n1D 1.4421, d19 0.9243. VI and VII (0.001 mole each) were treated with MeMgI according to the method of Treibs (C.A. 40, 53963) (millimoles MeMgI consumed after 3, 6, and 10 min. given): VI, 1.37, 1.47, 1.60; VII, 1.28, 1.32, 1.54. II (2 g.) and 1 g. Na heated 10 hrs. at 200° under N, treated with moist Et2O, and shaken with Et2O and dilute H2SO4, and the Et2O layer worked up yielded I, m. 34°. I (12 g.) in 18 cc. C5H5N treated slowly with cooling with 16.2 g. p-MeC6H4SO2Cl, kept 4 days at room temperature, poured into 113 g. 10% H2SO4, and filtered, and the crude product (11.6 g.) recrystd. from MeOH and then Me2CO yielded 5.9 g. I p-toluenesulfonate (VIII), m. 81°. The rates of hydrolysis were determined for the acid phthalates by treating 1.4516 g. ester with 0.05N H2SO4 (reaction time in hrs., and 2nd order rate consts. of IV and V given): I, 4.5, 0.55; 1.5, 4.8, 0.56; 2, 5.0, 0.59; 2.5, 5.2, 0.60; 3, 5.5, 0.60; 3.5, 5.6, 0.62; 4.5, 6.1, 0.64; 5.5, 6.5, 0.67. The solvolysis of VIII in MeOH (and EtOH) at reflux temperature was measured by titrating aliquots of a solution of 0.5971 g. VIII in 100 cc. absolute MeOH at time intervals; the olefin content in the titrated, neutral reaction mixture was determined by further titration with 0.1N Br; the first-order rate consts., k + 102 after 1, 2, 3, and 4 hrs., resp., for the solvolysis in MeOH were 3.61, 3.62, 3.59, and 3.68 with a half-life of the ester of 19.2 hrs.; the values obtained for the ethanolysis were 5.11, 5.5, 5.87, and 5.85 + 10-2, resp., with a half-life of the VIII of 12.5 hrs.

IT 67859-96-5

(Derived from data in the 6th Collective Formula Index
(1957-1961))

RN 67859-96-5 HCPLUS

CN Cyclohexanol, 3,3,5-trimethyl-, 1-acetate (CA INDEX NAME)



CC 10D (Organic Chemistry: Alicyclic Compounds)

IT 67859-96-5 93157-19-8

(Derived from data in the 6th Collective Formula Index
(1957-1961))

L4 ANSWER 8 OF 8 HCPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 1959:94507 HCPLUS Full-text

DOCUMENT NUMBER: 53:94507

ORIGINAL REFERENCE NO.: 53:17008c-i

TITLE:

Elimination reaction. X. Pyrolysis of xanthate and sulfite esters of erythro- and threo-3-(*p*-tolylthio)- and 3-(*p*-tolylsulfonyl)-2-butanol

AUTHOR(S):

Bordwell, F. G.; Landis, Phillip S.

CORPORATE SOURCE:

Northwestern Univ., Evanston, IL

SOURCE:

Journal of the American Chemical Society (1958),

80, 6383-6

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE:

Journal

LANGUAGE:

Unavailable

OTHER SOURCE(S):

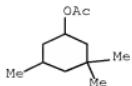
CASREACT 53:94507

AB The study of elimination reactions has been extended to the acyclic systems. dl-threo-3-(*p*-Tolylthio)-2-butanol added to a stirred suspension of K in dry C6H6, the mixture stirred 2 hrs. at room temperature and 2 hrs. at 50-5°, CS2 added, the solution refluxed 8 hrs., MeI added, the solution stirred overnight, filtered, washed with H2O, dried, the solvent evaporated, the crude xanthate pyrolyzed 30 min. at 200°, and the products distilled gave dl-threo-3-(*p*-tolylthio)-2-butyl S-Me xanthate (XIII), b0.1 135-47°. XIII oxidized with 30% H2O2 in HOAc gave the sulfone, m. 35-45°, identified by its infrared spectrum as cis-2-(*p*-tolylsulfonyl)-2-butene (XIV); the strong 14.7 μ peak of the trans isomer was absent. The dl-erythro-isomer (XV) of XIII, similarly prepared and pyrolyzed, gave on oxidation mostly trans-2-(*p*-tolylsulfonyl)-2-butene (XVI), m. 45-7°. dl-threo-3-(*p*-Tolylsulfonyl)-2-butyl S-Me xanthate (XVII) similarly prepared and pyrolyzed gave 58% XIV, b0.5 145-55°, and no more than 5% trans isomer. The dl-erythro isomer (XVIII) of XVII gave on pyrolysis an oil, b2 145-75°, on fractionation by chromatographing over silica gel, a mixture of 80% XIV and 20% XVI was identified by infrared analysis. Pyrolysis of 6.5 g. XVII and 2.0 g. XVI, gave 5.3 g. mixture containing approx. 40% XVI vs. the calculated 30%, if no rearrangement had occurred. threo- and erythro-3-(*p*-Tolylsulfonyl)-2-butanol were treated with K in C6H6, the suspension shaken with 10% HCl, the C6H6 layer separated, washed with H2O, dried, and the C6H6 evaporated. The infrared spectrum from the erythro isomer showed no threo present (absence of 2 strong doublets at 10.18, 10.38 and 10.85, 11.05 μ); the strong band at 9.98 μ characteristic of the erythro-alc. was absent in the recovered threo-alc. XVI refluxed 30 min. with tert-BuOH containing K, the cooled solution poured into H2O, and extracted with CHCl3 gave on evaporation of CHCl3 a mixture identified by infrared analysis as 80% XIV and 20% XVI; further treatment with K-containing tert-BuOH gave pure XIV. XIV was unchanged on similar treatment. Me erythro-3-(*p*-tolylthio)-2-butyl sulfite (XIX) pyrolyzed in vacuo at 200-20° gave 97% distillate; the latter, oxidized with H2O2 gave a solid, m. 35-43°, identified by infrared analysis as a mixture of 25% XVI and 75% XIV. The strong 14.7 μ band of the trans isomer did not occur in the pyrolysis product from the threo isomer of XIX. Me erythro-3-(*p*-tolylsulfonyl)-2-butyl sulfite (XX) heated 30 min. at 170° under N and the product distilled in vacuo gave a product, b0.4 160-4°; after chromatographing over silica gel a mixture of 15% XVI and 85% XIV was obtained. Pyrolysis of the threo isomer of XX gave 10% XVI and 90% XIV. Since stereoselective cis elimination occurred in the pyrolysis of XIII and XV, with the formation of XIV and XVI, while XVII and XVIII gave on pyrolysis only the more stable isomer, XIV, it is concluded that the mechanism is a stepwise one, involving a polar intermediate which can undergo rotation prior to forming olefin. XX and its threo isomer both gave XIV on pyrolysis, indicating a similar mechanism. An acid-catalyzed rearrangement of one of the olefins is believed responsible for the identity of pyrolysis products from XIII and its threo isomer.

IT 67859-96-5

(Derived from data in the 6th Collective Formula Index
(1957-1961))

RN 67859-96-5 HCPLUS
CN Cyclohexanol, 3,3,5-trimethyl-, 1-acetate (CA INDEX NAME)



CC 10D (Organic Chemistry: Alicyclic Compounds)
IT 67859-96-5 93157-19-8
(Derived from data in the 6th Collective Formula Index
(1957-1961))

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